

## Claims

- [c1] 1. A method to improve a CHTS experiment, comprising steps of:  
formulating an array of a mixture of at least two components;  
conducting an experiment on the array to produce results; and  
applying at least one Six Sigma technique to a step of the experiment  
to improve results of the experiment.
- [c2] 2. The method of claim 1, additionally comprising monitoring the step of  
formulating the array of a mixture.
- [c3] 3. The method of claim 1, additionally comprising monitoring the step of  
formulating the array of a mixture and identifying the step as an opportunity  
for a defect.
- [c4] 4. The method of claim 1, wherein the array of a mixture is formulated by  
delivering components of reactants to a well of an array plate.
- [c5] 5. The method of claim 1, wherein the array of a mixture is formulated by  
delivering components of reactants to a well of an array plate using a robotic  
dispenser.
- [c6] 6. The method of claim 1, wherein applying at least one Six Sigma technique  
includes identifying a defect opportunity.
- [c7] 7. The method of claim 1, wherein applying at least one Six Sigma technique  
includes identifying a defect opportunity selected from steps of monitoring a  
stock precursor solution, mixing an aliquot of the stock solution with an  
aliquot of another solution, delivering a mixture of the aliquots to a well of  
an array plate, effecting a condition of reaction on the mixture, detecting a  
result of the reaction and analyzing the result to determine either a lead or  
to determine a candidate library for reiterating the experiment.
- [c8] 8. The method of claim 1, comprising (A) an iteration of steps of (i)  
formulating an array of mixtures of at least two components; (ii) reacting the  
array mixtures; and (iii) evaluating a set of products of the reacting step and

(B) repeating the iteration of steps (i), (ii) and (iii) wherein components of a successive array of mixtures selected for a step (i) are chosen as a result of an evaluating step (iii) of a preceding iteration.

[c9] 9. The method of claim 1, wherein applying the Six Sigma technique comprises determining a Sigma value as equal to an absolute value function of a difference between average value of measurements on the system minus a nearest specification divided by a standard deviation of the measurements on the system.

[c10] 10. The method of claim 1, wherein applying the Six Sigma technique comprises determining a Sigma value as equal to per million occurrences of a ratio of number of defects of a product to number of opportunities for defect times number of units of the product.

[c11] 11. The method of claim 1, wherein applying at least one Six Sigma technique includes identifying a step of delivering stock solution to a well or substrate as a critical to quality defect opportunity.

[c12] 12. The method of claim 1, wherein applying at least one Six Sigma technique includes identifying a defect as a ternary mixture concentration that deviates more than  $(l/3 * \sqrt{3})$  from a design concentration where  $l$  is a height of an equilateral triangle of a graphic representation of the mixture.

[c13] 13. The method of claim 1, wherein applying at least one Six Sigma technique includes calculating a Sigma value equal to  $(l/3 * \sqrt{3}) / \sigma_p$  where  $l$  is a height of an equilateral triangle of a graphic representation of the mixture and  $\sigma_p$  is standard deviation.

[c14] 14. The method of claim 1, wherein the Six Sigma technique includes establishing a project goal Sigma value of at least 4.5.

[c15] 15. The method of claim 1, wherein the Six Sigma technique includes establishing a project goal Sigma value of at least 5.0.

[c16] 16. The method of claim 1, wherein the Six Sigma technique includes

establishing a project goal Sigma value of at least 5.5.

- [c17] 17. The method of claim 1, wherein the Six Sigma technique includes (1) selecting a point on a gradient representation of the mixture; (2) selecting a design concentration for each stock solution and an estimate of the standard deviation for each stock solution used to generate a mixture represented by the point; (3) determining an amount of each stock solution required to generate the mixture; (4) randomly selecting another stock concentration value from normal value distributions of concentration from the point mixture; (5) calculating a delivered concentration of components of a mixture resulting from mixing design amounts of stock solution; (6) calculating a distance between delivered concentration and the design concentration; and (7) counting a defect when the calculated distance exceeds  $1/3 * \sqrt{3}$ .
- [c18] 18. The method of claim 17, wherein steps (3) to (7) are repeated until at least 3 defects are counted.
- [c19] 19. The method of claim 17, wherein steps (3) to (7) are repeated until at least 10 defects are counted.
- [c20] 20. The method of claim 17, wherein steps (3) to (7) are repeated until 1,000,000 defect opportunities are counted.
- [c21] 21. The method of claim 17, wherein the mixture is a ternary, quaternary or pentanary mixture.
- [c22] 22. The method of claim 17, wherein steps (3) and (4) are determined according to formulas (III) through (VII) based on an assumption of no error in the stock solution concentration.
- [c23] 23. The method of claim 17, wherein the distance between delivered concentration and design concentration is calculated according to the formula (where SQRT is the square root function).
- [c24] 24. The method of claim 1, wherein the Six Sigma technique identifies at

least one of viscosity of stock solution, speed of withdrawal of solution from a stock solution vial, speed of addition to an array well and diameter of pipet tip as an area for improving Sigma of the formulating step.

- [c25] 25. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities.
- [c26] 26. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value.
- [c27] 27. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value by comparing the ratio to a Sigma chart.
- [c28] 28. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value by comparing the ratio to a Sigma chart stored in the data base of a processor.
- [c29] 29. The method of claim 1, wherein the Six Sigma technique includes calculating a ratio of defects/opportunities and the calculated ratio is normalized to a Sigma value corresponding to defects per million opportunities (DPMO).
- [c30] 30. The method of claim 1, wherein a low Sigma cause is identified and Sigma is improved by improving the low sigma cause.
- [c31] 31. The method of claim 1, wherein the components include a catalyst system comprising combinations of Group IVB, Group VIB and Lanthanide Group metal complexes.
- [c32] 32. The method of claim 1, wherein the components include a catalyst system comprising a Group VIII B metal.
- [c33] 33. The method of claim 1, wherein the components include a catalyst

system comprising palladium.

- [c34] 34. The method of claim 1, wherein the components include a catalyst system comprising a halide composition.
- [c35] 35. The method of claim 1, wherein the components include an inorganic co-catalyst.
- [c36] 36. The method of claim 1, wherein the components include a catalyst system that includes a combination of inorganic co-catalysts.
- [c37] 37. A method, comprising:
- identifying a reactant delivering step as an opportunity for a defect in a CHTS experiment;
  - measuring a number of units produced by the delivering step;
  - measuring defects in the units produced by the delivering step of the repeated CHTS; and
  - calculating a defects per unit for the delivering step.
- [c38] 38. The method of claim 37, wherein the CHTS experiment comprises an iteration of steps of simultaneously reacting a multiplicity of tagged reactants and identifying a multiplicity of tagged products of the reaction and evaluating products after completion of a single or repeated iteration.
- [c39] 39. The method of claim 37, wherein the CHTS experiment comprises effecting parallel chemical reactions of an array of reactant mixtures.
- [c40] 40. The method of claim 37, wherein the CHTS experiment is characterized by parallel reactions at a micro scale.
- [c41] 41. The method of claim 37, wherein the CHTS experiment comprises (A) an iteration of steps of (i) delivering mixtures of reactants to array wells; (ii) reacting the mixtures and (iii) evaluating a set of products of the reacting step and (B) repeating the iteration of steps (i), (ii) and (iii) wherein a successive mixture of reactants selected for a step (i) is chosen as a result of an evaluating step (iii) of a preceding iteration.

- [c42] 42. The method of claim 37, wherein the CHTS experiment comprises effecting parallel chemical reactions of an array of ternary reactant mixtures.
- [c43] 43. A method, comprising:
- identifying a reactant delivering step or stock formulating step as an opportunity for a defect in a mixture experiment;
  - measuring a number of units produced by the delivering step or formulating step;
  - measuring defects in the units produced by the delivering step or the formulating step; and
  - calculating a defects per unit for the delivering step or formulating step.
- [c44] 44. The method of claim 43, wherein the experiment is a ternary, quaternary or pentanary mixture experiment.
- [c45] 45. The method of claim 43, wherein the experiment is a ternary, mixture experiment.